



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:23 PM GMT

PDB ID : 1AIG
Title : PHOTOSYNTHETIC REACTION CENTER FROM RHODOBACTER SPHAEROIDES IN THE D+QB-CHARGE SEPARATED STATE
Authors : Stowell, M.H.B.; Mcphillips, T.M.; Soltis, S.M.; Rees, D.C.; Abresch, E.; Fehrer, G.
Deposited on : 1997-04-17
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

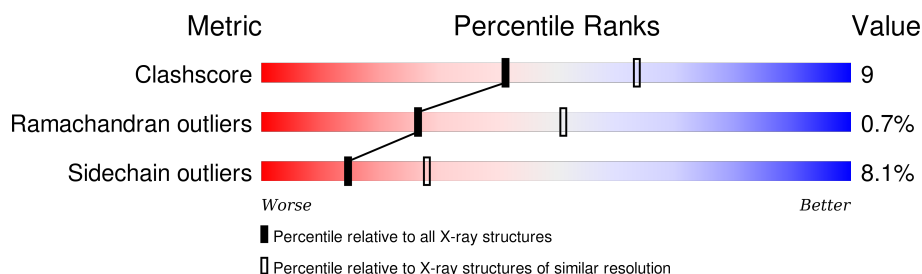
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	281	
1	N	281	
2	M	307	
2	O	307	
3	H	260	
3	P	260	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BCL	M	309	X	-	-	-
5	BCL	M	310	X	-	-	-
5	BCL	N	282	X	-	-	-
5	BCL	O	309	X	-	-	-
6	BPH	L	284	X	-	-	-
6	BPH	L	285	X	-	-	-
6	BPH	N	285	X	-	-	-
6	BPH	O	310	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14138 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PHOTOSYNTHETIC REACTION CENTER (L SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			
1	N	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER (M SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	299	Total	C	N	O	S	0	0	0
			2390	1597	391	392	10			
2	O	299	Total	C	N	O	S	0	0	0
			2390	1597	391	392	10			

- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER (H SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	248	Total	C	N	O	S	0	0	0
			1883	1204	322	347	10			
3	P	248	Total	C	N	O	S	0	0	0
			1883	1204	322	347	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	8	GLN	GLY	CONFLICT	UNP P11846
P	8	GLN	GLY	CONFLICT	UNP P11846

- Molecule 4 is FE (II) ION (three-letter code: FE2) (formula: Fe).

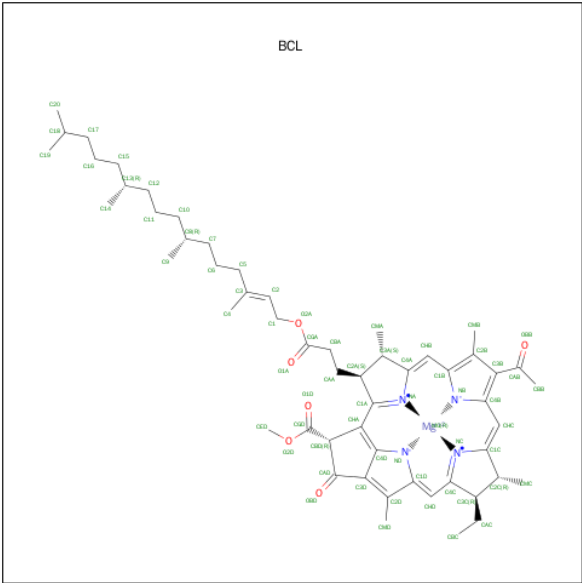
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	1	Total	Fe	0	0
			1	1		

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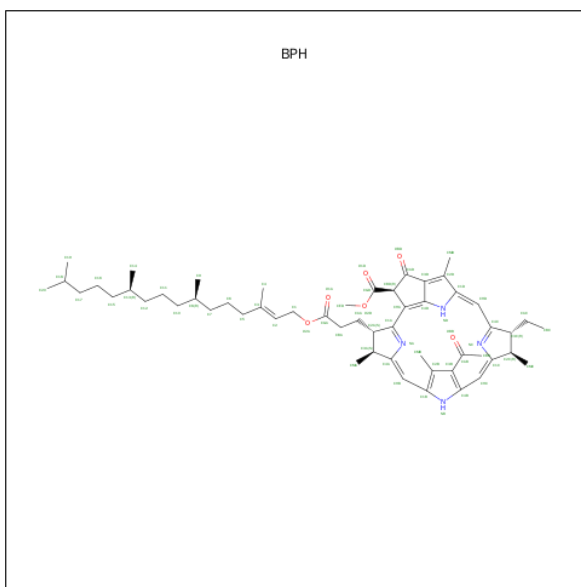
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total	Fe	0	0
			1	1		

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



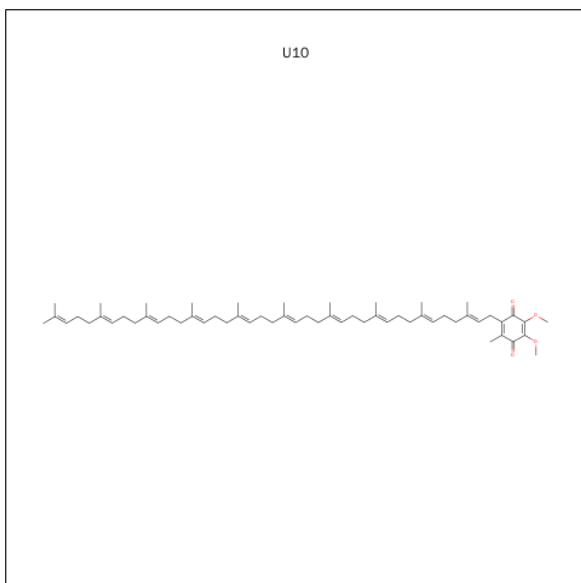
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	N	1	Total	C	Mg	N	O	12	0
			66	55	1	4	6		
5	N	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	O	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	N	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 6 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	14	0
			65	55	4	6		
6	L	1	Total	C	N	O	0	0
			65	55	4	6		
6	O	1	Total	C	N	O	0	0
			65	55	4	6		
6	N	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 7 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	C	O	0	0
			63	59	4		
7	L	1	Total	C	O	0	0
			63	59	4		
7	O	1	Total	C	O	0	0
			63	59	4		
7	N	1	Total	C	O	19	0
			63	59	4		

- Molecule 8 is water.

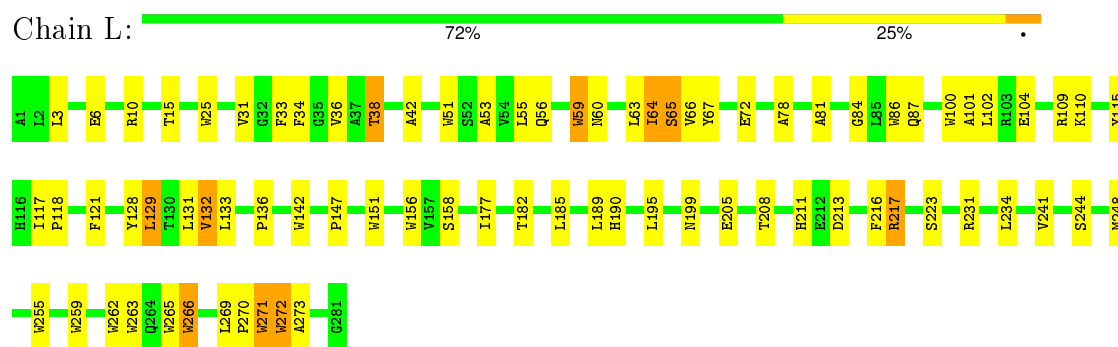
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	13	Total	O	0	0
			13	13		
8	L	19	Total	O	0	0
			19	19		
8	M	21	Total	O	0	0
			21	21		
8	N	13	Total	O	0	0
			13	13		
8	O	15	Total	O	0	0
			15	15		
8	P	5	Total	O	0	0
			5	5		

3 Residue-property plots

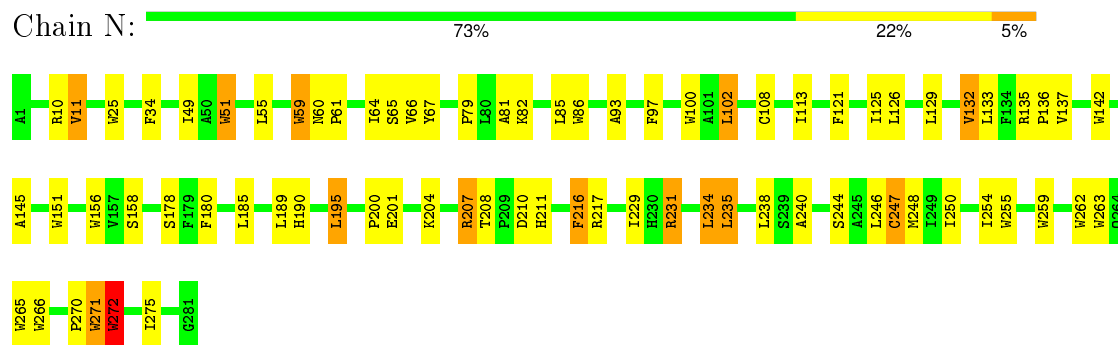
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

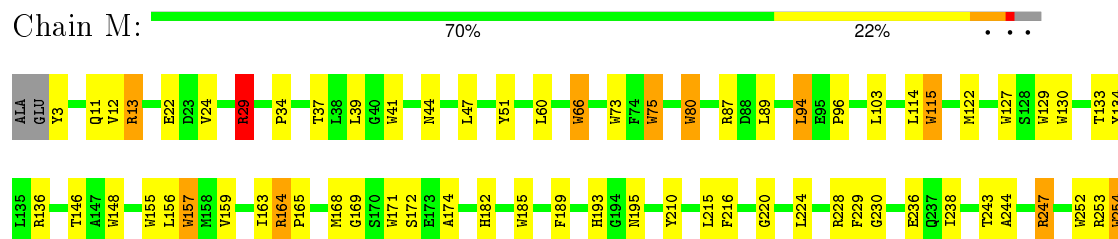
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER (L SUBUNIT)



• Molecule 1: PHOTOSYNTHETIC REACTION CENTER (L SUBUNIT)



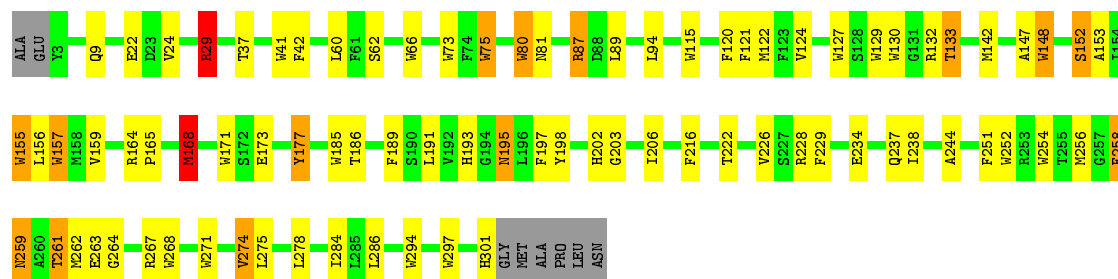
• Molecule 2: PHOTOSYNTHETIC REACTION CENTER (M SUBUNIT)





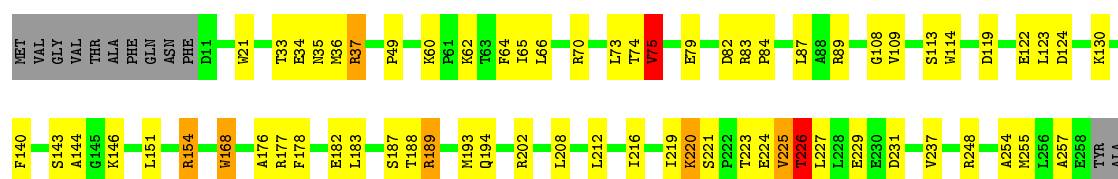
• Molecule 2: PHOTOSYNTHETIC REACTION CENTER (M SUBUNIT)

Chain O: 70% 22% 5% ..



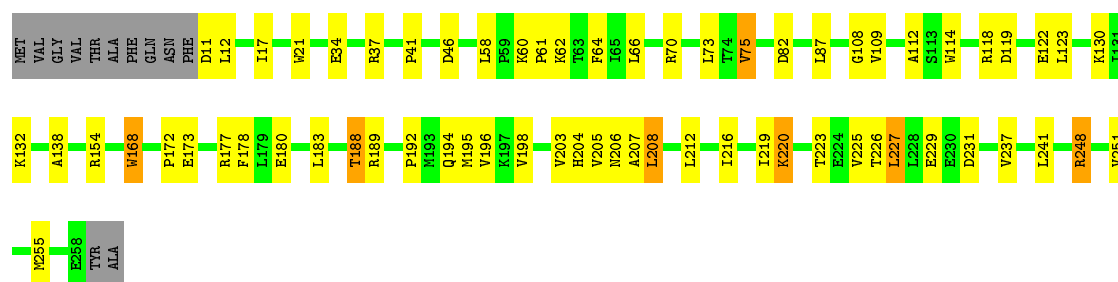
• Molecule 3: PHOTOSYNTHETIC REACTION CENTER (H SUBUNIT)

Chain H: 70% 23% .. 5%



• Molecule 3: PHOTOSYNTHETIC REACTION CENTER (H SUBUNIT)

Chain P: 70% 23% • 5%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	140.10Å 140.10Å 271.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60	Depositor
% Data completeness (in resolution range)	88.0 (30.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	X-PLOR 3.89	Depositor
R, R_{free}	0.215 , 0.299	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14138	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, BPH, FE2, U10

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	L	0.87	0/2320	1.65	69/3175 (2.2%)
1	N	0.85	0/2320	1.59	53/3175 (1.7%)
2	M	0.90	0/2482	1.68	81/3389 (2.4%)
2	O	0.89	0/2482	1.60	68/3389 (2.0%)
3	H	0.76	0/1931	1.44	23/2627 (0.9%)
3	P	0.75	0/1931	1.38	15/2627 (0.6%)
All	All	0.85	0/13466	1.57	309/18382 (1.7%)

There are no bond length outliers.

All (309) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	217	ARG	NE-CZ-NH1	9.66	125.13	120.30
2	M	41	TRP	CD1-CG-CD2	9.54	113.93	106.30
2	O	297	TRP	CD1-CG-CD2	9.42	113.83	106.30
1	N	231	ARG	NE-CZ-NH1	9.41	125.01	120.30
3	H	37	ARG	NE-CZ-NH2	-9.33	115.64	120.30
1	L	51	TRP	CD1-CG-CD2	9.28	113.72	106.30
2	M	254	TRP	CD1-CG-CD2	9.26	113.70	106.30
2	O	157	TRP	CD1-CG-CD2	9.12	113.60	106.30
1	N	25	TRP	CD1-CG-CD2	9.09	113.57	106.30
1	N	51	TRP	CD1-CG-CD2	9.07	113.56	106.30
1	N	59	TRP	CD1-CG-CD2	9.05	113.54	106.30
1	L	217	ARG	NE-CZ-NH2	-9.01	115.79	120.30
2	M	171	TRP	CD1-CG-CD2	8.90	113.42	106.30
2	O	271	TRP	CD1-CG-CD2	8.81	113.35	106.30
2	M	297	TRP	CD1-CG-CD2	8.74	113.29	106.30
1	N	142	TRP	CD1-CG-CD2	8.66	113.23	106.30
2	M	185	TRP	CD1-CG-CD2	8.64	113.21	106.30
1	N	100	TRP	CD1-CG-CD2	8.63	113.20	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	130	TRP	CD1-CG-CD2	8.58	113.17	106.30
1	L	86	TRP	CD1-CG-CD2	8.57	113.16	106.30
2	O	171	TRP	CD1-CG-CD2	8.55	113.14	106.30
2	M	80	TRP	CD1-CG-CD2	8.51	113.11	106.30
1	L	59	TRP	CD1-CG-CD2	8.51	113.10	106.30
1	L	142	TRP	CD1-CG-CD2	8.46	113.06	106.30
2	M	66	TRP	CD1-CG-CD2	8.32	112.96	106.30
1	N	25	TRP	CE2-CD2-CG	-8.28	100.68	107.30
1	L	255	TRP	CD1-CG-CD2	8.26	112.91	106.30
1	L	272	TRP	CD1-CG-CD2	8.22	112.88	106.30
1	N	151	TRP	CD1-CG-CD2	8.22	112.88	106.30
2	M	171	TRP	CE2-CD2-CG	-8.20	100.74	107.30
1	L	142	TRP	CE2-CD2-CG	-8.19	100.75	107.30
2	M	75	TRP	CD1-CG-CD2	8.19	112.85	106.30
3	P	21	TRP	CD1-CG-CD2	8.18	112.84	106.30
2	O	185	TRP	CD1-CG-CD2	8.15	112.82	106.30
2	O	148	TRP	CD1-CG-CD2	8.14	112.81	106.30
1	N	59	TRP	CE2-CD2-CG	-8.13	100.79	107.30
2	O	75	TRP	CD1-CG-CD2	8.13	112.80	106.30
2	O	148	TRP	CE2-CD2-CG	-8.13	100.80	107.30
1	L	151	TRP	CD1-CG-CD2	8.12	112.79	106.30
2	M	127	TRP	CD1-CG-CD2	8.10	112.78	106.30
2	M	148	TRP	CE2-CD2-CG	-8.08	100.84	107.30
1	N	263	TRP	CD1-CG-CD2	8.07	112.76	106.30
2	M	41	TRP	CE2-CD2-CG	-8.06	100.85	107.30
2	O	129	TRP	CD1-CG-CD2	8.05	112.74	106.30
2	M	148	TRP	CD1-CG-CD2	8.02	112.71	106.30
2	O	29	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	L	59	TRP	CE2-CD2-CG	-7.99	100.91	107.30
1	N	262	TRP	CD1-CG-CD2	7.98	112.68	106.30
3	H	168	TRP	CD1-CG-CD2	7.97	112.67	106.30
1	N	259	TRP	CD1-CG-CD2	7.93	112.64	106.30
1	L	51	TRP	CE2-CD2-CG	-7.92	100.97	107.30
2	M	254	TRP	CE2-CD2-CG	-7.89	100.99	107.30
2	M	80	TRP	CE2-CD2-CG	-7.88	100.99	107.30
2	O	297	TRP	CE2-CD2-CG	-7.88	101.00	107.30
2	O	294	TRP	CD1-CG-CD2	7.88	112.60	106.30
1	N	142	TRP	CE2-CD2-CG	-7.82	101.05	107.30
2	M	155	TRP	CE2-CD2-CG	-7.81	101.05	107.30
2	M	129	TRP	CD1-CG-CD2	7.81	112.55	106.30
2	O	294	TRP	CE2-CD2-CG	-7.79	101.07	107.30
1	L	231	ARG	NE-CZ-NH1	7.79	124.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	86	TRP	CD1-CG-CD2	7.77	112.52	106.30
1	N	255	TRP	CD1-CG-CD2	7.77	112.51	106.30
1	N	51	TRP	CE2-CD2-CG	-7.76	101.09	107.30
3	H	114	TRP	CD1-CG-CD2	7.76	112.51	106.30
3	P	21	TRP	CE2-CD2-CG	-7.76	101.09	107.30
3	P	168	TRP	CD1-CG-CD2	7.76	112.50	106.30
1	L	259	TRP	CD1-CG-CD2	7.75	112.50	106.30
3	H	37	ARG	NE-CZ-NH1	7.75	124.18	120.30
1	L	263	TRP	CE2-CD2-CG	-7.74	101.11	107.30
2	O	157	TRP	CE2-CD2-CG	-7.71	101.13	107.30
1	L	151	TRP	CE2-CD2-CG	-7.69	101.15	107.30
3	P	114	TRP	CD1-CG-CD2	7.69	112.45	106.30
2	M	185	TRP	CE2-CD2-CG	-7.69	101.15	107.30
2	M	297	TRP	CE2-CD2-CG	-7.68	101.16	107.30
2	M	3	TYR	CB-CG-CD2	-7.67	116.40	121.00
2	O	271	TRP	CE2-CD2-CG	-7.66	101.17	107.30
2	O	75	TRP	CE2-CD2-CG	-7.66	101.18	107.30
2	O	171	TRP	CE2-CD2-CG	-7.65	101.18	107.30
1	N	151	TRP	CE2-CD2-CG	-7.62	101.20	107.30
1	L	156	TRP	CD1-CG-CD2	7.60	112.38	106.30
1	N	263	TRP	CE2-CD2-CG	-7.59	101.22	107.30
1	L	266	TRP	CE2-CD2-CG	-7.59	101.23	107.30
1	N	86	TRP	CE2-CD2-CG	-7.58	101.24	107.30
1	L	266	TRP	CD1-CG-CD2	7.56	112.35	106.30
1	L	86	TRP	CE2-CD2-CG	-7.55	101.26	107.30
3	P	118	ARG	NE-CZ-NH1	7.52	124.06	120.30
2	M	157	TRP	CD1-CG-CD2	7.52	112.32	106.30
2	M	75	TRP	CE2-CD2-CG	-7.52	101.28	107.30
1	N	217	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	N	100	TRP	CE2-CD2-CG	-7.50	101.30	107.30
2	O	185	TRP	CE2-CD2-CG	-7.50	101.30	107.30
2	M	155	TRP	CD1-CG-CD2	7.49	112.29	106.30
1	L	259	TRP	CE2-CD2-CG	-7.48	101.32	107.30
2	M	127	TRP	CE2-CD2-CG	-7.47	101.32	107.30
2	O	66	TRP	CD1-CG-CD2	7.47	112.28	106.30
1	L	271	TRP	CE2-CD2-CG	-7.45	101.34	107.30
1	L	265	TRP	CD1-CG-CD2	7.45	112.26	106.30
2	O	80	TRP	CD1-CG-CD2	7.44	112.25	106.30
2	O	130	TRP	CE2-CD2-CG	-7.44	101.35	107.30
2	M	129	TRP	CE2-CD2-CG	-7.43	101.36	107.30
2	O	252	TRP	CD1-CG-CD2	7.41	112.23	106.30
1	N	259	TRP	CE2-CD2-CG	-7.41	101.38	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	263	TRP	CD1-CG-CD2	7.40	112.22	106.30
3	H	168	TRP	CE2-CD2-CG	-7.38	101.39	107.30
2	M	294	TRP	CE2-CD2-CG	-7.37	101.40	107.30
1	N	265	TRP	CD1-CG-CD2	7.37	112.20	106.30
1	L	255	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	N	262	TRP	CE2-CD2-CG	-7.36	101.41	107.30
2	O	41	TRP	CD1-CG-CD2	7.36	112.19	106.30
1	L	100	TRP	CD1-CG-CD2	7.35	112.18	106.30
1	N	255	TRP	CE2-CD2-CG	-7.34	101.43	107.30
2	O	80	TRP	CE2-CD2-CG	-7.33	101.43	107.30
2	M	268	TRP	CD1-CG-CD2	7.31	112.15	106.30
3	P	114	TRP	CE2-CD2-CG	-7.31	101.45	107.30
1	N	272	TRP	CD1-CG-CD2	7.31	112.15	106.30
2	M	73	TRP	CD1-CG-CD2	7.30	112.14	106.30
1	L	265	TRP	CE2-CD2-CG	-7.29	101.47	107.30
2	O	115	TRP	CD1-CG-CD2	7.28	112.13	106.30
1	L	100	TRP	CE2-CD2-CG	-7.28	101.47	107.30
1	L	25	TRP	CE2-CD2-CG	-7.28	101.48	107.30
2	M	73	TRP	CE2-CD2-CG	-7.27	101.49	107.30
3	H	114	TRP	CE2-CD2-CG	-7.24	101.51	107.30
3	P	168	TRP	CE2-CD2-CG	-7.22	101.52	107.30
2	M	148	TRP	CG-CD2-CE3	7.21	140.39	133.90
2	O	115	TRP	CE2-CD2-CG	-7.20	101.54	107.30
3	H	89	ARG	NE-CZ-NH1	7.20	123.90	120.30
2	M	130	TRP	CD1-CG-CD2	7.19	112.05	106.30
1	N	266	TRP	CD1-CG-CD2	7.18	112.05	106.30
2	O	41	TRP	CE2-CD2-CG	-7.17	101.57	107.30
1	L	271	TRP	CD1-CG-CD2	7.16	112.03	106.30
2	O	129	TRP	CE2-CD2-CG	-7.16	101.57	107.30
2	O	268	TRP	CD1-CG-CD2	7.16	112.03	106.30
1	N	271	TRP	CA-CB-CG	7.15	127.29	113.70
1	N	266	TRP	CE2-CD2-CG	-7.15	101.58	107.30
2	M	268	TRP	CE2-CD2-CG	-7.14	101.59	107.30
2	M	271	TRP	CD1-CG-CD2	7.14	112.01	106.30
2	M	271	TRP	CE2-CD2-CG	-7.12	101.60	107.30
2	M	134	TYR	CB-CG-CD2	-7.12	116.73	121.00
2	O	66	TRP	CE2-CD2-CG	-7.11	101.62	107.30
2	O	252	TRP	CE2-CD2-CG	-7.10	101.62	107.30
3	H	21	TRP	CE2-CD2-CG	-7.10	101.62	107.30
2	O	127	TRP	CE2-CD2-CG	-7.09	101.63	107.30
2	O	268	TRP	CE2-CD2-CG	-7.08	101.64	107.30
2	M	66	TRP	CE2-CD2-CG	-7.06	101.65	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	252	TRP	CE2-CD2-CG	-7.03	101.68	107.30
2	O	148	TRP	CG-CD2-CE3	7.02	140.22	133.90
2	M	157	TRP	CE2-CD2-CG	-7.01	101.69	107.30
2	M	294	TRP	CD1-CG-CD2	6.96	111.87	106.30
1	N	265	TRP	CE2-CD2-CG	-6.95	101.74	107.30
2	O	254	TRP	CE2-CD2-CG	-6.95	101.74	107.30
1	L	25	TRP	CD1-CG-CD2	6.94	111.86	106.30
2	M	115	TRP	CE2-CD2-CG	-6.93	101.75	107.30
1	L	272	TRP	CE2-CD2-CG	-6.93	101.76	107.30
1	N	156	TRP	CE2-CD2-CG	-6.92	101.77	107.30
2	M	130	TRP	CE2-CD2-CG	-6.91	101.77	107.30
1	L	156	TRP	CE2-CD2-CG	-6.90	101.78	107.30
1	N	271	TRP	CE2-CD2-CG	-6.85	101.82	107.30
2	O	155	TRP	CE2-CD2-CG	-6.84	101.83	107.30
2	O	127	TRP	CD1-CG-CD2	6.81	111.75	106.30
2	O	73	TRP	CE2-CD2-CG	-6.78	101.88	107.30
2	M	171	TRP	CG-CD2-CE3	6.73	139.96	133.90
1	L	262	TRP	CE2-CD2-CG	-6.71	101.93	107.30
1	L	262	TRP	CD1-CG-CD2	6.66	111.62	106.30
2	M	171	TRP	CB-CG-CD1	-6.64	118.36	127.00
2	O	155	TRP	CD1-CG-CD2	6.61	111.58	106.30
2	O	254	TRP	CD1-CG-CD2	6.58	111.56	106.30
2	M	247	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	N	156	TRP	CD1-CG-CD2	6.56	111.55	106.30
3	H	225	VAL	CB-CA-C	-6.54	98.97	111.40
1	N	272	TRP	CE2-CD2-CG	-6.54	102.07	107.30
2	M	115	TRP	CD1-CG-CD2	6.54	111.53	106.30
2	O	148	TRP	CB-CG-CD1	-6.49	118.56	127.00
2	M	148	TRP	CB-CG-CD1	-6.46	118.60	127.00
1	L	151	TRP	CG-CD2-CE3	6.44	139.70	133.90
2	M	252	TRP	CD1-CG-CD2	6.41	111.43	106.30
1	L	86	TRP	CG-CD2-CE3	6.40	139.66	133.90
1	L	265	TRP	CG-CD2-CE3	6.37	139.63	133.90
1	N	25	TRP	CG-CD2-CE3	6.36	139.62	133.90
2	M	136	ARG	NE-CZ-NH1	6.34	123.47	120.30
2	O	185	TRP	CG-CD2-CE3	6.34	139.60	133.90
1	L	271	TRP	CG-CD2-CE3	6.31	139.58	133.90
3	P	255	MET	CA-CB-CG	6.28	123.98	113.30
1	L	265	TRP	CB-CG-CD1	-6.28	118.84	127.00
3	H	21	TRP	CD1-CG-CD2	6.28	111.32	106.30
2	M	261	THR	CA-CB-CG2	6.27	121.17	112.40
3	P	118	ARG	NE-CZ-NH2	-6.26	117.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	136	ARG	NE-CZ-NH2	-6.25	117.17	120.30
3	H	248	ARG	NE-CZ-NH1	6.20	123.40	120.30
2	O	73	TRP	CD1-CG-CD2	6.20	111.26	106.30
1	L	271	TRP	CB-CG-CD1	-6.18	118.96	127.00
1	L	142	TRP	CG-CD2-CE3	6.17	139.45	133.90
1	L	59	TRP	CG-CD2-CE3	6.16	139.44	133.90
3	H	237	VAL	CG1-CB-CG2	-6.13	101.09	110.90
2	O	259	ASN	N-CA-C	6.13	127.54	111.00
1	L	25	TRP	CG-CD2-CE3	6.12	139.41	133.90
1	L	142	TRP	CB-CG-CD1	-6.11	119.06	127.00
2	M	259	ASN	N-CA-C	6.09	127.44	111.00
3	H	89	ARG	NE-CZ-NH2	-6.08	117.26	120.30
2	M	254	TRP	CG-CD1-NE1	-6.07	104.03	110.10
1	L	151	TRP	CB-CG-CD1	-6.06	119.12	127.00
3	H	220	LYS	CA-CB-CG	6.05	126.70	113.40
1	N	86	TRP	CG-CD2-CE3	6.01	139.31	133.90
1	L	266	TRP	CB-CG-CD1	-5.98	119.23	127.00
2	M	13	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	N	263	TRP	CG-CD2-CE3	5.98	139.28	133.90
1	L	100	TRP	CG-CD2-CE3	5.96	139.26	133.90
3	H	21	TRP	CG-CD2-CE3	5.96	139.26	133.90
1	N	59	TRP	CG-CD2-CE3	5.95	139.26	133.90
2	O	185	TRP	CB-CG-CD1	-5.95	119.27	127.00
1	N	271	TRP	CD1-CG-CD2	5.95	111.06	106.30
1	L	271	TRP	CA-CB-CG	5.94	124.99	113.70
2	O	157	TRP	CG-CD1-NE1	-5.91	104.19	110.10
1	L	25	TRP	CB-CG-CD1	-5.91	119.31	127.00
3	P	248	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	L	266	TRP	CG-CD2-CE3	5.91	139.22	133.90
2	M	51	TYR	CB-CG-CD2	-5.90	117.46	121.00
1	L	86	TRP	CG-CD1-NE1	-5.90	104.20	110.10
2	M	41	TRP	CG-CD2-CE3	5.89	139.20	133.90
1	N	25	TRP	CB-CG-CD1	-5.85	119.40	127.00
2	M	258	PHE	CA-C-N	5.81	129.98	117.20
2	O	168	MET	CG-SD-CE	-5.81	90.91	100.20
2	O	87	ARG	NE-CZ-NH1	5.79	123.20	120.30
2	M	29	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	L	244	SER	N-CA-CB	-5.77	101.85	110.50
1	N	51	TRP	CG-CD1-NE1	-5.77	104.33	110.10
1	L	51	TRP	CG-CD1-NE1	-5.75	104.35	110.10
2	M	87	ARG	NE-CZ-NH1	5.75	123.18	120.30
2	O	297	TRP	CG-CD1-NE1	-5.75	104.35	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	67	TYR	CB-CG-CD1	-5.72	117.57	121.00
1	N	263	TRP	CB-CG-CD1	-5.72	119.56	127.00
2	M	168	MET	CG-SD-CE	-5.71	91.06	100.20
3	H	154	ARG	NE-CZ-NH2	-5.71	117.45	120.30
2	O	294	TRP	CG-CD2-CE3	5.69	139.02	133.90
2	M	41	TRP	CB-CG-CD1	-5.67	119.63	127.00
2	M	41	TRP	CG-CD1-NE1	-5.67	104.43	110.10
2	M	185	TRP	CG-CD1-NE1	-5.67	104.43	110.10
2	M	247	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	N	86	TRP	CB-CG-CD1	-5.59	119.73	127.00
2	O	171	TRP	CG-CD1-NE1	-5.59	104.51	110.10
1	L	86	TRP	CB-CG-CD1	-5.57	119.76	127.00
2	O	274	VAL	CA-CB-CG2	-5.56	102.56	110.90
2	M	297	TRP	CG-CD1-NE1	-5.53	104.57	110.10
2	O	294	TRP	CB-CG-CD1	-5.53	119.81	127.00
2	O	171	TRP	CG-CD2-CE3	5.47	138.82	133.90
2	M	164	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	N	25	TRP	CG-CD1-NE1	-5.45	104.65	110.10
2	M	258	PHE	N-CA-C	5.45	125.71	111.00
3	H	202	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	L	65	SER	CA-C-N	5.44	129.17	117.20
1	N	100	TRP	CG-CD1-NE1	-5.42	104.67	110.10
2	M	171	TRP	CG-CD1-NE1	-5.42	104.68	110.10
2	O	171	TRP	CB-CG-CD1	-5.42	119.95	127.00
2	M	185	TRP	CG-CD2-CE3	5.41	138.77	133.90
1	N	59	TRP	CG-CD1-NE1	-5.41	104.69	110.10
2	O	256	MET	CA-CB-CG	5.40	122.48	113.30
1	L	59	TRP	CB-CG-CD1	-5.40	119.98	127.00
1	L	255	TRP	CG-CD1-NE1	-5.39	104.70	110.10
1	L	272	TRP	CG-CD1-NE1	-5.39	104.71	110.10
3	P	21	TRP	CG-CD2-CE3	5.39	138.75	133.90
2	M	80	TRP	CG-CD2-CE3	5.38	138.74	133.90
2	O	130	TRP	CG-CD1-NE1	-5.37	104.73	110.10
2	O	297	TRP	CB-CG-CD1	-5.34	120.06	127.00
1	N	132	VAL	N-CA-CB	-5.33	99.77	111.50
1	L	72	GLU	CA-CB-CG	5.31	125.09	113.40
3	P	208	LEU	CA-CB-CG	5.31	127.51	115.30
2	M	129	TRP	CG-CD1-NE1	-5.29	104.81	110.10
2	O	155	TRP	CB-CG-CD1	-5.28	120.14	127.00
2	M	80	TRP	CB-CG-CD1	-5.27	120.15	127.00
2	O	261	THR	CA-CB-CG2	5.26	119.76	112.40
2	M	254	TRP	CG-CD2-CE3	5.26	138.63	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	226	THR	N-CA-CB	-5.25	100.32	110.30
3	P	177	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	L	263	TRP	CG-CD2-CE3	5.24	138.62	133.90
1	N	271	TRP	CG-CD2-CE3	5.22	138.60	133.90
2	M	294	TRP	CG-CD2-CE3	5.21	138.59	133.90
2	M	185	TRP	CB-CG-CD1	-5.21	120.23	127.00
3	H	21	TRP	CB-CG-CD1	-5.21	120.23	127.00
1	L	72	GLU	CB-CA-C	-5.19	100.01	110.40
1	N	266	TRP	CB-CG-CD1	-5.19	120.25	127.00
2	M	267	ARG	NE-CZ-NH1	5.19	122.89	120.30
2	O	271	TRP	CG-CD1-NE1	-5.18	104.92	110.10
2	M	297	TRP	CB-CG-CD1	-5.17	120.27	127.00
3	H	75	VAL	N-CA-CB	-5.17	100.11	111.50
2	O	258	PHE	N-CA-C	5.17	124.96	111.00
1	L	100	TRP	CB-CG-CD1	-5.17	120.28	127.00
1	N	59	TRP	CB-CG-CD1	-5.16	120.29	127.00
1	N	142	TRP	CG-CD1-NE1	-5.16	104.94	110.10
2	M	297	TRP	CG-CD2-CE3	5.15	138.54	133.90
1	L	265	TRP	CG-CD1-NE1	-5.15	104.95	110.10
3	H	87	LEU	CA-CB-CG	5.14	127.12	115.30
3	P	132	LYS	CA-CB-CG	5.14	124.70	113.40
2	M	80	TRP	CG-CD1-NE1	-5.14	104.96	110.10
1	L	156	TRP	CG-CD1-NE1	-5.13	104.97	110.10
2	M	155	TRP	CB-CG-CD1	-5.13	120.33	127.00
2	M	253	ARG	NE-CZ-NH1	5.12	122.86	120.30
2	O	129	TRP	CG-CD1-NE1	-5.11	104.99	110.10
3	P	220	LYS	CA-CB-CG	5.10	124.62	113.40
1	N	10	ARG	NE-CZ-NH1	5.09	122.85	120.30
2	O	132	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	L	263	TRP	CB-CG-CD1	-5.08	120.40	127.00
2	O	80	TRP	CG-CD2-CE3	5.07	138.47	133.90
2	O	177	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	L	10	ARG	NE-CZ-NH1	5.06	122.83	120.30
2	O	80	TRP	CB-CG-CD1	-5.06	120.43	127.00
1	L	59	TRP	CG-CD1-NE1	-5.05	105.05	110.10
3	H	74	THR	CA-C-N	-5.04	106.11	117.20
1	N	265	TRP	CB-CG-CD1	-5.02	120.47	127.00
2	M	75	TRP	CG-CD1-NE1	-5.01	105.09	110.10
3	H	189	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2232	0	2187	39	0
1	N	2232	0	2187	40	0
2	M	2390	0	2304	36	0
2	O	2390	0	2304	47	0
3	H	1883	0	1895	30	0
3	P	1883	0	1895	30	0
4	M	1	0	0	0	0
4	O	1	0	0	0	0
5	L	132	0	148	11	0
5	M	132	0	148	12	0
5	N	198	0	222	18	0
5	O	66	0	74	9	0
6	L	130	0	152	11	0
6	N	65	0	76	7	0
6	O	65	0	76	3	0
7	L	63	0	90	4	0
7	M	63	0	90	1	0
7	N	63	0	90	6	0
7	O	63	0	90	2	0
8	H	13	0	0	3	0
8	L	19	0	0	4	0
8	M	21	0	0	0	0
8	N	13	0	0	0	0
8	O	15	0	0	1	0
8	P	5	0	0	0	0
All	All	14138	0	14028	238	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (238) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:275:LEU:O	2:M:279:THR:HB	1.86	0.75
5:N:282:BCL:HBB3	5:O:309:BCL:H41	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:284:BCL:HED2	2:O:203:GLY:HA3	1.72	0.70
2:M:261:THR:HG22	2:M:264:GLY:H	1.55	0.70
3:H:226:THR:HG22	3:H:229:GLU:H	1.55	0.70
1:L:241:VAL:HG21	6:L:285:BPH:HAC2	1.74	0.70
6:L:285:BPH:HBB3	6:L:285:BPH:HHC	1.74	0.68
2:O:197:PHE:HZ	5:O:309:BCL:HBB2	1.60	0.67
1:L:55:LEU:HD13	1:L:81:ALA:HB2	1.76	0.67
6:L:285:BPH:H142	6:L:285:BPH:H102	1.78	0.65
1:N:229:ILE:HD13	7:N:286:U10:H102	1.79	0.64
6:N:285:BPH:HHC	6:N:285:BPH:CBB	2.28	0.64
2:M:122:MET:HE3	2:M:157:TRP:HE1	1.63	0.63
5:M:309:BCL:HMB1	5:M:309:BCL:HBB2	1.80	0.63
1:L:60:ASN:O	1:L:64:ILE:HG22	1.98	0.63
2:M:133:THR:HG23	2:M:146:THR:HG22	1.81	0.62
1:N:93:ALA:HA	6:N:285:BPH:H9C2	1.80	0.62
1:N:135:ARG:HD2	1:N:248:MET:O	1.99	0.62
1:L:53:ALA:HB2	1:L:64:ILE:HG13	1.83	0.61
5:O:309:BCL:H42	6:O:310:BPH:HBB2	1.83	0.60
3:P:154:ARG:HE	3:P:204:HIS:HD2	1.48	0.60
2:O:275:LEU:HD23	2:O:278:LEU:HD23	1.84	0.59
2:O:122:MET:HE3	2:O:157:TRP:HE1	1.67	0.59
1:L:65:SER:HB2	8:L:289:HOH:O	2.02	0.59
2:O:197:PHE:CZ	5:O:309:BCL:HBB2	2.38	0.59
1:L:208:THR:H	1:L:211:HIS:HD2	1.51	0.59
2:O:122:MET:HE1	2:O:177:TYR:HE1	1.68	0.58
3:P:168:TRP:HB2	3:P:178:PHE:HB2	1.85	0.58
2:M:157:TRP:HB2	5:M:310:BCL:H71	1.85	0.58
3:P:70:ARG:NH2	3:P:123:LEU:HD13	2.19	0.58
1:N:195:LEU:HD11	2:O:267:ARG:HG2	1.86	0.57
3:H:183:LEU:HD11	3:H:189:ARG:HD2	1.86	0.57
3:H:119:ASP:OD1	3:H:226:THR:HG21	2.04	0.57
6:N:285:BPH:HHC	6:N:285:BPH:HBB2	1.87	0.57
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.85	0.57
2:O:155:TRP:O	2:O:159:VAL:HG23	2.05	0.57
3:H:189:ARG:HD3	3:H:216:ILE:HB	1.86	0.57
2:M:103:LEU:HG	2:M:169:GLY:O	2.03	0.57
1:N:185:LEU:HD13	6:O:310:BPH:ND	2.20	0.56
5:O:309:BCL:HBB3	5:O:309:BCL:HHC	1.88	0.56
1:N:11:VAL:HG23	3:P:87:LEU:HD11	1.87	0.55
2:O:153:ALA:HB2	6:O:310:BPH:HAC1	1.88	0.55
2:M:39:LEU:HD12	2:M:47:LEU:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:42:ALA:HB2	6:L:285:BPH:H4C1	1.89	0.55
2:O:9:GLN:NE2	3:P:198:VAL:H	2.04	0.54
1:N:97:PHE:HB3	1:N:125:ILE:HG12	1.89	0.54
7:N:286:U10:H322	2:O:42:PHE:CD1	2.43	0.54
2:O:228:ARG:HA	3:P:194:GLN:CG	2.37	0.53
5:N:282:BCL:HBB1	2:O:157:TRP:HD1	1.73	0.53
5:N:282:BCL:HHC	5:N:282:BCL:HBB2	1.88	0.53
2:M:230:GLY:HA2	8:H:267:HOH:O	2.07	0.53
2:O:228:ARG:HA	3:P:194:GLN:HG3	1.91	0.53
2:O:237:GLN:HB2	2:O:262:MET:HG2	1.90	0.53
3:H:34:GLU:O	3:H:37:ARG:HG3	2.08	0.53
3:H:37:ARG:HB3	3:H:75:VAL:HG13	1.90	0.53
5:M:310:BCL:OBB	5:M:310:BCL:HHC	2.09	0.53
1:N:178:SER:HA	5:N:282:BCL:HBA2	1.89	0.53
1:L:131:LEU:HD21	1:L:248:MET:HG3	1.90	0.53
3:P:226:THR:HG22	3:P:229:GLU:H	1.72	0.53
5:L:282:BCL:CBB	5:L:282:BCL:HMB1	2.39	0.53
2:O:261:THR:HG22	2:O:263:GLU:H	1.73	0.53
1:L:56:GLN:HE22	1:L:64:ILE:HA	1.73	0.52
1:N:201:GLU:HB2	1:N:204:LYS:HD2	1.90	0.52
1:L:208:THR:H	1:L:211:HIS:CD2	2.27	0.52
3:H:176:ALA:HB1	3:H:193:MET:HG3	1.90	0.52
3:P:183:LEU:HD11	3:P:189:ARG:HD2	1.90	0.52
1:N:108:CYS:HG	2:O:251:PHE:HE2	1.57	0.52
3:H:219:ILE:HG23	3:H:229:GLU:OE1	2.10	0.51
1:L:177:ILE:HG12	5:L:282:BCL:HMB3	1.92	0.51
2:O:24:VAL:HG11	2:O:29:ARG:NH1	2.26	0.51
5:L:282:BCL:H151	6:L:285:BPH:H2	1.92	0.51
2:O:9:GLN:HE22	3:P:198:VAL:H	1.59	0.51
1:N:246:LEU:O	1:N:250:ILE:HB	2.11	0.51
5:N:282:BCL:HHC	5:N:282:BCL:CBB	2.41	0.51
3:H:119:ASP:HA	3:H:226:THR:HG23	1.93	0.50
2:O:234:GLU:O	2:O:238:ILE:HG13	2.10	0.50
2:M:189:PHE:O	2:M:193:HIS:HD2	1.95	0.50
1:N:208:THR:H	1:N:211:HIS:CD2	2.28	0.50
1:L:84:GLY:HA2	1:L:87:GLN:HE21	1.76	0.50
6:L:285:BPH:HHC	6:L:285:BPH:CBB	2.41	0.50
1:L:269:LEU:O	1:L:273:ALA:HB2	2.12	0.50
2:M:260:ALA:HA	3:H:35:ASN:HB3	1.94	0.50
5:O:309:BCL:CBB	5:O:309:BCL:HHC	2.42	0.49
3:H:108:GLY:O	3:H:113:SER:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:13:ARG:O	3:H:140:PHE:HA	2.12	0.49
1:N:185:LEU:CD2	5:N:282:BCL:H43	2.42	0.49
6:L:285:BPH:HBB2	2:M:210:TYR:HB3	1.94	0.49
3:P:119:ASP:HA	3:P:226:THR:HG23	1.94	0.49
3:P:130:LYS:NZ	3:P:173:GLU:HG3	2.27	0.49
3:P:62:LYS:HE2	3:P:64:PHE:CZ	2.47	0.49
2:M:260:ALA:HB1	3:H:35:ASN:OD1	2.12	0.49
3:P:41:PRO:HG3	3:P:58:LEU:HD11	1.95	0.49
1:N:81:ALA:H	1:N:85:LEU:HB2	1.78	0.49
2:M:24:VAL:HG11	2:M:29:ARG:NH1	2.28	0.49
5:M:309:BCL:H41	5:M:309:BCL:H61	1.61	0.48
3:P:154:ARG:HH21	3:P:204:HIS:CD2	2.31	0.48
7:L:286:U10:H162	5:M:309:BCL:H92	1.96	0.48
3:H:62:LYS:HE2	3:H:64:PHE:CZ	2.48	0.48
1:L:213:ASP:O	1:L:217:ARG:HB2	2.13	0.48
2:O:261:THR:HG22	2:O:264:GLY:H	1.77	0.48
3:P:37:ARG:O	3:P:75:VAL:HG22	2.13	0.48
3:P:207:ALA:HB1	3:P:237:VAL:O	2.14	0.48
1:L:185:LEU:HD13	6:L:284:BPH:ND	2.29	0.47
1:N:208:THR:OG1	1:N:211:HIS:HD2	1.97	0.47
7:N:286:U10:H71	7:N:286:U10:H1M1	1.58	0.47
7:L:286:U10:H252	7:L:286:U10:H201	1.97	0.47
1:L:182:THR:OG1	5:M:309:BCL:H11	2.14	0.47
1:L:190:HIS:HA	7:L:286:U10:O2	2.14	0.47
1:N:136:PRO:HG2	1:N:145:ALA:HB2	1.96	0.47
3:H:168:TRP:HB2	3:H:178:PHE:HB2	1.96	0.47
1:L:33:PHE:O	1:L:36:VAL:HG22	2.14	0.47
3:P:196:VAL:HG12	3:P:205:VAL:HG22	1.97	0.47
2:M:96:PRO:HB2	2:M:172:SER:HA	1.96	0.47
2:M:157:TRP:HD1	5:M:309:BCL:HBB1	1.79	0.47
3:H:177:ARG:NH1	8:H:267:HOH:O	2.46	0.46
3:P:37:ARG:NH2	3:P:62:LYS:HB2	2.30	0.46
1:N:231:ARG:O	1:N:235:LEU:HB2	2.15	0.46
2:O:202:HIS:HD2	5:O:309:BCL:HED2	1.80	0.46
3:P:130:LYS:NZ	3:P:172:PRO:HG2	2.30	0.46
1:N:79:PRO:HG2	1:N:82:LYS:HB3	1.96	0.46
1:L:110:LYS:HD2	2:M:254:TRP:CZ3	2.51	0.46
2:M:94:LEU:HD13	2:M:115:TRP:HA	1.96	0.46
1:N:180:PHE:CE2	1:N:240:ALA:HB1	2.51	0.46
7:L:286:U10:H501	7:L:286:U10:H563	1.96	0.46
8:L:295:HOH:O	3:H:130:LYS:HE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:121:PHE:CZ	6:N:285:BPH:HBA2	2.50	0.46
1:N:190:HIS:HA	7:N:286:U10:O2	2.16	0.46
5:N:283:BCL:CBB	5:N:283:BCL:HMB1	2.46	0.46
5:N:283:BCL:CGA	5:N:284:BCL:HBC1	2.46	0.46
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.51	0.46
3:P:189:ARG:HD3	3:P:216:ILE:HB	1.98	0.46
3:H:66:LEU:HB3	3:H:70:ARG:HB2	1.97	0.46
2:O:168:MET:HG2	2:O:173:GLU:HG3	1.99	0.46
3:H:154:ARG:NH2	8:H:270:HOH:O	2.48	0.45
2:O:222:THR:O	2:O:226:VAL:HG22	2.17	0.45
1:L:3:LEU:HB2	1:L:6:GLU:HB2	1.97	0.45
5:N:282:BCL:H3C	2:O:186:THR:OG1	2.16	0.45
1:N:272:TRP:CE2	2:O:87:ARG:HB3	2.51	0.45
5:O:309:BCL:HMB1	5:O:309:BCL:OBB	2.16	0.45
6:L:284:BPH:HMA3	5:M:310:BCL:H192	1.99	0.45
3:P:119:ASP:HA	3:P:226:THR:CG2	2.47	0.45
1:L:205:GLU:HG2	3:H:65:ILE:HG22	1.98	0.45
1:N:34:PHE:CE1	1:N:102:LEU:HD23	2.51	0.45
3:H:182:GLU:HA	3:H:187:SER:O	2.16	0.45
1:L:185:LEU:CD2	5:M:309:BCL:H52	2.47	0.45
2:M:236:GLU:HG3	3:H:122:GLU:CD	2.37	0.45
3:H:219:ILE:HG21	3:H:224:GLU:O	2.16	0.45
7:N:286:U10:H322	2:O:42:PHE:CG	2.51	0.45
2:M:238:ILE:HG23	2:M:263:GLU:HB2	1.99	0.45
2:O:122:MET:HE1	2:O:177:TYR:CE1	2.49	0.45
2:M:75:TRP:HB3	2:M:80:TRP:CE3	2.51	0.45
2:O:206:ILE:HG23	5:O:309:BCL:HMB3	1.98	0.45
1:L:129:LEU:HG	1:L:133:LEU:HD23	1.99	0.44
1:L:199:ASN:HD21	2:M:267:ARG:HH12	1.64	0.44
1:L:60:ASN:HB3	1:L:63:LEU:HD12	2.00	0.44
8:L:300:HOH:O	3:H:79:GLU:HB2	2.17	0.44
5:N:284:BCL:CBB	5:N:284:BCL:HMB1	2.48	0.44
5:N:283:BCL:H11	5:N:284:BCL:HBC3	2.00	0.44
5:N:284:BCL:HMB1	5:N:284:BCL:HBB2	1.99	0.43
2:O:237:GLN:CB	2:O:262:MET:HG2	2.48	0.43
2:O:164:ARG:HB3	2:O:165:PRO:HD3	2.00	0.43
3:P:122:GLU:HB2	3:P:227:LEU:HD11	2.00	0.43
1:N:244:SER:OG	5:N:283:BCL:HBA2	2.18	0.43
1:N:275:ILE:HG21	2:O:81:ASN:ND2	2.33	0.43
1:N:234:LEU:HD22	1:N:238:LEU:HD22	2.00	0.43
5:L:282:BCL:H2C	5:M:310:BCL:H2C	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:283:BCL:H122	6:N:285:BPH:H3A	2.01	0.43
5:N:283:BCL:HHC	5:N:283:BCL:OBB	2.19	0.43
5:L:282:BCL:HBD	5:L:283:BCL:HAC1	2.00	0.43
5:L:283:BCL:HMB1	5:L:283:BCL:HBB2	2.00	0.43
3:P:108:GLY:HA2	3:P:112:ALA:O	2.19	0.43
5:L:283:BCL:HMD2	5:M:310:BCL:HBB3	2.01	0.43
1:L:147:PRO:HB2	8:L:289:HOH:O	2.18	0.43
2:O:62:SER:HB3	2:O:121:PHE:O	2.19	0.43
1:N:93:ALA:HA	6:N:285:BPH:C9	2.48	0.42
2:O:164:ARG:HD2	2:O:284:ILE:HG22	2.01	0.42
2:M:165:PRO:HG2	2:M:174:ALA:HB2	2.00	0.42
1:L:78:ALA:H	1:L:87:GLN:HE22	1.66	0.42
1:L:34:PHE:O	1:L:38:THR:HB	2.19	0.42
7:O:311:U10:H421	7:O:311:U10:H401	1.85	0.42
1:L:121:PHE:CZ	6:L:285:BPH:HBA2	2.54	0.42
5:L:283:BCL:H172	6:L:285:BPH:H142	2.01	0.42
2:M:228:ARG:HA	3:H:194:GLN:CG	2.49	0.42
3:P:241:LEU:HA	3:P:248:ARG:NH2	2.34	0.42
1:N:200:PRO:HB3	1:N:207:ARG:HD3	2.02	0.42
5:N:284:BCL:HMD1	2:O:206:ILE:HD13	2.00	0.42
5:L:282:BCL:HAA2	5:L:283:BCL:HBC1	2.01	0.42
1:L:266:TRP:O	1:L:269:LEU:HB2	2.19	0.42
2:M:11:GLN:HB2	3:H:144:ALA:HB3	2.02	0.42
1:L:158:SER:HA	5:L:282:BCL:HBC1	2.01	0.42
2:M:13:ARG:HB2	3:H:143:SER:HB3	2.02	0.42
2:O:152:SER:OG	2:O:274:VAL:HG13	2.19	0.42
2:M:215:LEU:HD13	7:M:311:U10:H153	2.01	0.42
2:M:159:VAL:HA	2:M:163:ILE:HB	2.02	0.42
1:N:180:PHE:CD2	1:N:240:ALA:HB1	2.55	0.42
1:N:60:ASN:HA	1:N:61:PRO:HD3	1.75	0.42
2:O:229:PHE:HB2	2:O:244:ALA:HB2	2.02	0.42
3:P:192:PRO:HB2	3:P:195:MET:HB2	2.02	0.41
3:P:130:LYS:HZ1	3:P:173:GLU:HG3	1.84	0.41
1:L:128:TYR:O	1:L:132:VAL:HB	2.20	0.41
8:O:322:HOH:O	3:P:34:GLU:HG3	2.19	0.41
2:M:220:GLY:O	2:M:224:LEU:HG	2.20	0.41
1:L:115:TYR:O	1:L:118:PRO:HG2	2.20	0.41
1:N:135:ARG:HB3	1:N:136:PRO:HD3	2.02	0.41
2:O:261:THR:HG22	2:O:263:GLU:N	2.35	0.41
3:H:254:ALA:O	3:H:257:ALA:HB3	2.20	0.41
2:M:34:PRO:O	2:M:47:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:164:ARG:HB3	2:M:165:PRO:HD3	2.02	0.41
1:N:207:ARG:HG2	2:O:142:MET:HG2	2.02	0.41
1:L:109:ARG:HG3	1:L:115:TYR:HE1	1.86	0.41
1:L:117:ILE:H	1:L:117:ILE:HD12	1.86	0.41
2:O:120:PHE:O	2:O:124:VAL:HG23	2.20	0.41
3:H:33:THR:O	3:H:36:MET:HB2	2.19	0.41
1:N:55:LEU:HD13	1:N:81:ALA:HB2	2.02	0.41
1:N:65:SER:HG	1:N:67:TYR:HE1	1.66	0.41
3:P:180:GLU:OE2	3:P:188:THR:HG21	2.21	0.41
2:M:75:TRP:HB3	2:M:80:TRP:CZ3	2.56	0.41
3:P:206:ASN:O	3:P:248:ARG:NH1	2.54	0.41
2:O:189:PHE:O	2:O:193:HIS:HD2	2.04	0.41
2:O:75:TRP:HB3	2:O:80:TRP:CE3	2.56	0.41
1:N:133:LEU:O	1:N:137:VAL:HG23	2.20	0.41
2:M:243:THR:O	2:M:247:ARG:HG3	2.20	0.41
1:N:216:PHE:CG	7:N:286:U10:H72	2.56	0.41
1:N:113:ILE:HD11	2:O:251:PHE:CD2	2.56	0.41
1:N:247:CYS:O	1:N:250:ILE:HG22	2.21	0.41
3:H:146:LYS:NZ	3:H:151:LEU:HD21	2.36	0.41
1:L:15:THR:N	1:L:109:ARG:HH12	2.19	0.40
2:O:202:HIS:CE1	2:O:206:ILE:HD11	2.57	0.40
1:L:185:LEU:HD23	5:M:309:BCL:H52	2.03	0.40
2:O:258:PHE:HE1	7:O:311:U10:H211	1.86	0.40
1:N:51:TRP:CE3	1:N:51:TRP:HA	2.57	0.40
2:O:133:THR:CG2	2:O:147:ALA:HA	2.52	0.40
1:N:238:LEU:HD12	6:N:285:BPH:CBC	2.51	0.40
2:O:195:ASN:HB3	2:O:198:TYR:HD2	1.86	0.40
5:N:284:BCL:H141	5:N:284:BCL:H18	2.03	0.40
5:L:282:BCL:CGA	5:L:283:BCL:HBC1	2.51	0.40
1:L:101:ALA:O	1:L:104:GLU:HB2	2.20	0.40
1:L:223:SER:O	2:M:44:ASN:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	279/281 (99%)	261 (94%)	14 (5%)	4 (1%)	14	28
1	N	279/281 (99%)	261 (94%)	15 (5%)	3 (1%)	17	36
2	M	297/307 (97%)	284 (96%)	11 (4%)	2 (1%)	26	51
2	O	297/307 (97%)	284 (96%)	11 (4%)	2 (1%)	26	51
3	H	246/260 (95%)	238 (97%)	8 (3%)	0	100	100
3	P	246/260 (95%)	238 (97%)	7 (3%)	1 (0%)	39	65
All	All	1644/1696 (97%)	1566 (95%)	66 (4%)	12 (1%)	26	51

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	270	PRO
2	M	259	ASN
2	O	259	ASN
1	L	271	TRP
2	M	195	ASN
1	N	271	TRP
2	O	195	ASN
1	N	270	PRO
1	L	66	VAL
3	P	138	ALA
1	N	66	VAL
1	L	31	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	220/220 (100%)	208 (94%)	12 (6%)	27	51
1	N	220/220 (100%)	201 (91%)	19 (9%)	13	25
2	M	235/240 (98%)	218 (93%)	17 (7%)	18	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	O	235/240 (98%)	220 (94%)	15 (6%)	22	43
3	H	200/209 (96%)	179 (90%)	21 (10%)	8	16
3	P	200/209 (96%)	178 (89%)	22 (11%)	8	14
All	All	1310/1338 (98%)	1204 (92%)	106 (8%)	15	28

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	38	THR
1	L	59	TRP
1	L	64	ILE
1	L	102	LEU
1	L	129	LEU
1	L	132	VAL
1	L	136	PRO
1	L	189	LEU
1	L	195	LEU
1	L	216	PHE
1	L	234	LEU
1	L	272	TRP
2	M	12	VAL
2	M	22	GLU
2	M	29	ARG
2	M	37	THR
2	M	60	LEU
2	M	89	LEU
2	M	94	LEU
2	M	114	LEU
2	M	156	LEU
2	M	182	HIS
2	M	216	PHE
2	M	259	ASN
2	M	261	THR
2	M	279	THR
2	M	286	LEU
2	M	292	ASP
2	M	300	ASN
3	H	49	PRO
3	H	60	LYS
3	H	73	LEU
3	H	75	VAL

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Mol	Chain	Res	Type
3	H	82	ASP
3	H	83	ARG
3	H	84	PRO
3	H	109	VAL
3	H	123	LEU
3	H	124	ASP
3	H	188	THR
3	H	208	LEU
3	H	212	LEU
3	H	220	LYS
3	H	221	SER
3	H	223	THR
3	H	225	VAL
3	H	226	THR
3	H	227	LEU
3	H	231	ASP
3	H	255	MET
1	N	11	VAL
1	N	49	ILE
1	N	59	TRP
1	N	64	ILE
1	N	102	LEU
1	N	126	LEU
1	N	129	LEU
1	N	132	VAL
1	N	158	SER
1	N	189	LEU
1	N	195	LEU
1	N	207	ARG
1	N	210	ASP
1	N	216	PHE
1	N	234	LEU
1	N	235	LEU
1	N	247	CYS
1	N	254	ILE
1	N	272	TRP
2	O	22	GLU
2	O	29	ARG
2	O	37	THR
2	O	60	LEU
2	O	89	LEU
2	O	94	LEU

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Mol	Chain	Res	Type
2	O	133	THR
2	O	148	TRP
2	O	152	SER
2	O	156	LEU
2	O	168	MET
2	O	191	LEU
2	O	216	PHE
2	O	286	LEU
2	O	301	HIS
3	P	11	ASP
3	P	12	LEU
3	P	17	ILE
3	P	46	ASP
3	P	60	LYS
3	P	61	PRO
3	P	66	LEU
3	P	73	LEU
3	P	75	VAL
3	P	82	ASP
3	P	109	VAL
3	P	188	THR
3	P	203	VAL
3	P	208	LEU
3	P	212	LEU
3	P	219	ILE
3	P	220	LYS
3	P	223	THR
3	P	225	VAL
3	P	227	LEU
3	P	231	ASP
3	P	251	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	56	GLN
1	L	87	GLN
1	L	199	ASN
1	L	211	HIS
2	M	9	GLN
2	M	145	HIS
2	M	193	HIS

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Mol	Chain	Res	Type
3	H	204	HIS
1	N	87	GLN
1	N	159	ASN
1	N	183	ASN
1	N	199	ASN
1	N	211	HIS
2	O	9	GLN
2	O	11	GLN
2	O	145	HIS
2	O	193	HIS
3	P	199	GLN
3	P	204	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	BCL	L	282	1	53,74,74	1.12	6 (11%)	57,115,115	1.48	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BCL	L	283	1	53,74,74	1.11	5 (9%)	57,115,115	1.75	12 (21%)
6	BPH	L	284	-	64,70,70	1.21	5 (7%)	73,101,101	1.68	11 (15%)
6	BPH	L	285	-	64,70,70	1.10	6 (9%)	73,101,101	1.75	17 (23%)
7	U10	L	286	-	63,63,63	1.87	16 (25%)	76,79,79	1.42	9 (11%)
5	BCL	M	309	2	53,74,74	1.11	5 (9%)	57,115,115	1.89	13 (22%)
5	BCL	M	310	2	53,74,74	1.05	5 (9%)	57,115,115	1.70	10 (17%)
7	U10	M	311	-	63,63,63	1.86	15 (23%)	76,79,79	1.37	11 (14%)
5	BCL	N	282	2	53,74,74	1.25	8 (15%)	57,115,115	1.83	11 (19%)
5	BCL	N	283	1,5	53,74,74	1.12	6 (11%)	57,115,115	1.72	16 (28%)
5	BCL	N	284	1	53,74,74	1.13	6 (11%)	57,115,115	1.68	14 (24%)
6	BPH	N	285	-	64,70,70	1.13	6 (9%)	73,101,101	1.98	13 (17%)
7	U10	N	286	-	63,63,63	1.83	15 (23%)	76,79,79	1.58	9 (11%)
5	BCL	O	309	2,5	53,74,74	1.10	5 (9%)	57,115,115	1.51	10 (17%)
6	BPH	O	310	-	64,70,70	1.18	7 (10%)	73,101,101	1.89	12 (16%)
7	U10	O	311	-	63,63,63	1.72	14 (22%)	76,79,79	1.26	9 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BCL	L	282	1	-	0/37/137/137	0/0/9/9
5	BCL	L	283	1	-	0/37/137/137	0/0/9/9
6	BPH	L	284	-	2/2/18/22	0/54/105/105	0/1/6/6
6	BPH	L	285	-	1/1/18/22	0/54/105/105	0/1/6/6
7	U10	L	286	-	-	0/63/87/87	0/1/1/1
5	BCL	M	309	2	2/2/21/25	0/37/137/137	0/0/9/9
5	BCL	M	310	2	2/2/21/25	0/37/137/137	0/0/9/9
7	U10	M	311	-	-	0/63/87/87	0/1/1/1
5	BCL	N	282	2	2/2/21/25	0/37/137/137	0/0/9/9
5	BCL	N	283	1,5	-	0/37/137/137	0/0/9/9
5	BCL	N	284	1	-	0/37/137/137	0/0/9/9
6	BPH	N	285	-	1/1/18/22	0/54/105/105	0/1/6/6
7	U10	N	286	-	-	0/63/87/87	0/1/1/1
5	BCL	O	309	2,5	1/1/21/25	0/37/137/137	0/0/9/9
6	BPH	O	310	-	1/1/18/22	0/54/105/105	0/1/6/6
7	U10	O	311	-	-	0/63/87/87	0/1/1/1

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	286	U10	C7-C8	-4.75	1.43	1.50
7	M	311	U10	C7-C8	-4.59	1.43	1.50
6	N	285	BPH	C3D-CAD	-4.29	1.38	1.46
6	O	310	BPH	C3D-CAD	-4.26	1.38	1.46
7	N	286	U10	C7-C8	-4.19	1.44	1.50
6	L	284	BPH	C3D-CAD	-4.18	1.38	1.46
5	L	282	BCL	O2D-CGD	-4.13	1.22	1.33
7	N	286	U10	C32-C33	-4.10	1.39	1.50
5	O	309	BCL	O2D-CGD	-3.80	1.23	1.33
5	L	283	BCL	O2D-CGD	-3.70	1.23	1.33
6	L	285	BPH	C3D-CAD	-3.65	1.39	1.46
5	N	282	BCL	O2D-CGD	-3.49	1.24	1.33
6	L	284	BPH	O2D-CGD	-3.38	1.24	1.33
5	N	283	BCL	O2D-CGD	-3.36	1.24	1.33
7	L	286	U10	C3-C2	-3.30	1.39	1.48
5	N	284	BCL	O2D-CGD	-3.27	1.24	1.33
5	O	309	BCL	C3B-CAB	-3.26	1.40	1.49
6	L	284	BPH	O2A-CGA	-3.26	1.23	1.33
5	M	309	BCL	O2D-CGD	-3.20	1.25	1.33
6	N	285	BPH	C1B-C2B	-3.19	1.38	1.45
5	M	309	BCL	C3D-CAD	-3.18	1.36	1.45
6	O	310	BPH	O2A-CGA	-3.15	1.23	1.33
6	N	285	BPH	O2D-CGD	-3.15	1.25	1.33
5	N	283	BCL	O2A-CGA	-3.09	1.23	1.33
6	L	285	BPH	C1B-C2B	-3.07	1.39	1.45
7	N	286	U10	C4-C5	-3.06	1.40	1.48
5	M	310	BCL	O2D-CGD	-3.04	1.25	1.33
6	L	285	BPH	O2D-CGD	-3.03	1.25	1.33
7	O	311	U10	C3-C2	-3.03	1.40	1.48
5	N	283	BCL	CAA-C2A	-3.02	1.48	1.54
6	O	310	BPH	C1B-C2B	-3.02	1.39	1.45
6	L	285	BPH	O2A-CGA	-2.99	1.24	1.33
5	L	283	BCL	C3D-CAD	-2.97	1.37	1.45
5	M	309	BCL	O2A-CGA	-2.93	1.24	1.33
7	O	311	U10	C4-C5	-2.93	1.40	1.48
6	O	310	BPH	O2D-CGD	-2.92	1.25	1.33
5	N	282	BCL	O2A-CGA	-2.89	1.24	1.33
5	L	282	BCL	C3B-CAB	-2.88	1.41	1.49
6	N	285	BPH	O2A-CGA	-2.86	1.24	1.33
7	M	311	U10	C3-C2	-2.85	1.40	1.48
5	O	309	BCL	O2A-CGA	-2.85	1.24	1.33
6	L	284	BPH	C1B-C2B	-2.83	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	286	U10	C3-C2	-2.83	1.40	1.48
5	L	282	BCL	O2A-CGA	-2.80	1.24	1.33
7	L	286	U10	C4-C5	-2.78	1.40	1.48
5	M	310	BCL	C3D-CAD	-2.76	1.38	1.45
5	M	310	BCL	O2A-CGA	-2.76	1.25	1.33
7	M	311	U10	C4-C5	-2.71	1.41	1.48
5	L	283	BCL	O2A-CGA	-2.60	1.25	1.33
5	L	283	BCL	C3B-CAB	-2.54	1.42	1.49
5	O	309	BCL	C3D-CAD	-2.44	1.38	1.45
5	M	310	BCL	C3B-CAB	-2.38	1.42	1.49
5	N	284	BCL	O2A-CGA	-2.36	1.26	1.33
7	L	286	U10	C12-C13	-2.32	1.44	1.50
5	N	284	BCL	C3B-CAB	-2.30	1.42	1.49
5	N	284	BCL	C3D-CAD	-2.29	1.39	1.45
5	M	309	BCL	C3B-CAB	-2.26	1.42	1.49
6	L	285	BPH	C3A-C2A	-2.22	1.47	1.54
6	N	285	BPH	C3B-CAB	-2.21	1.39	1.46
5	N	283	BCL	C3D-CAD	-2.18	1.39	1.45
7	M	311	U10	C27-C28	-2.16	1.44	1.50
7	L	286	U10	C6-C5	-2.14	1.40	1.46
5	N	282	BCL	C3A-C2A	-2.12	1.48	1.54
6	O	310	BPH	C3B-C4B	-2.10	1.38	1.43
5	N	283	BCL	C3B-CAB	-2.07	1.43	1.49
5	L	282	BCL	C2C-C3C	-2.04	1.48	1.54
5	N	282	BCL	C3B-CAB	-2.01	1.43	1.49
5	L	282	BCL	CAA-C2A	-2.01	1.50	1.54
5	N	282	BCL	C3D-CAD	-2.00	1.40	1.45
7	N	286	U10	C35-C34	2.05	1.55	1.50
6	O	310	BPH	CHA-C1A	2.07	1.42	1.37
5	N	282	BCL	CAA-CBA	2.09	1.59	1.52
6	L	285	BPH	CHC-C1C	2.11	1.40	1.36
7	L	286	U10	C6-C1	2.11	1.40	1.35
7	L	286	U10	C53-C54	2.19	1.39	1.32
7	N	286	U10	C53-C54	2.21	1.39	1.32
6	N	285	BPH	C2-C3	2.26	1.37	1.33
7	O	311	U10	C53-C54	2.26	1.39	1.32
5	N	284	BCL	CAA-CBA	2.42	1.60	1.52
7	L	286	U10	C8-C9	2.44	1.37	1.33
7	O	311	U10	C7-C6	2.47	1.55	1.51
7	N	286	U10	C33-C34	2.47	1.37	1.33
7	M	311	U10	C8-C9	2.48	1.37	1.33
7	M	311	U10	C6-C1	2.50	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	311	U10	C53-C54	2.55	1.40	1.32
7	L	286	U10	C13-C14	2.64	1.38	1.33
7	O	311	U10	C13-C14	2.80	1.38	1.33
7	N	286	U10	C6-C1	2.84	1.41	1.35
5	M	309	BCL	C2-C3	2.84	1.38	1.33
5	L	283	BCL	C2-C3	2.94	1.38	1.33
6	L	284	BPH	C2-C3	2.96	1.38	1.33
5	N	284	BCL	C2-C3	2.97	1.38	1.33
6	O	310	BPH	C2-C3	2.98	1.38	1.33
7	M	311	U10	C28-C29	2.99	1.38	1.33
7	O	311	U10	C6-C1	3.00	1.42	1.35
5	M	310	BCL	C2-C3	3.04	1.38	1.33
5	N	282	BCL	CAA-C2A	3.04	1.60	1.54
5	N	283	BCL	C2-C3	3.07	1.39	1.33
7	O	311	U10	C48-C49	3.10	1.39	1.33
5	L	282	BCL	C2-C3	3.11	1.39	1.33
5	O	309	BCL	C2-C3	3.13	1.39	1.33
7	O	311	U10	C33-C34	3.13	1.39	1.33
7	M	311	U10	C23-C24	3.14	1.39	1.33
7	N	286	U10	C48-C49	3.15	1.39	1.33
7	O	311	U10	C18-C19	3.20	1.39	1.33
7	O	311	U10	C38-C39	3.25	1.39	1.33
7	L	286	U10	C43-C44	3.28	1.39	1.33
7	L	286	U10	C18-C19	3.29	1.39	1.33
7	N	286	U10	C43-C44	3.32	1.39	1.33
7	M	311	U10	C13-C14	3.33	1.39	1.33
7	O	311	U10	C43-C44	3.37	1.39	1.33
7	N	286	U10	C13-C14	3.39	1.39	1.33
7	O	311	U10	C23-C24	3.40	1.39	1.33
7	N	286	U10	C23-C24	3.47	1.39	1.33
7	N	286	U10	C38-C39	3.47	1.39	1.33
7	M	311	U10	C18-C19	3.50	1.39	1.33
7	O	311	U10	C8-C9	3.51	1.39	1.33
7	L	286	U10	C33-C34	3.57	1.40	1.33
7	M	311	U10	C33-C34	3.62	1.40	1.33
7	L	286	U10	C38-C39	3.63	1.40	1.33
7	N	286	U10	C18-C19	3.77	1.40	1.33
7	N	286	U10	C28-C29	3.88	1.40	1.33
7	M	311	U10	C48-C49	3.90	1.40	1.33
7	L	286	U10	C48-C49	4.00	1.40	1.33
5	N	282	BCL	C2-C3	4.01	1.40	1.33
7	M	311	U10	C43-C44	4.07	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	311	U10	C38-C39	4.11	1.41	1.33
7	L	286	U10	C28-C29	4.12	1.41	1.33
7	O	311	U10	C28-C29	4.14	1.41	1.33
7	L	286	U10	C23-C24	4.22	1.41	1.33

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	310	BPH	O1D-CGD-CBD	-7.29	114.17	124.62
6	N	285	BPH	O1D-CGD-CBD	-6.07	115.92	124.62
5	M	309	BCL	O1D-CGD-CBD	-5.32	117.00	124.62
6	L	285	BPH	C4D-C3D-C2D	-5.04	100.57	107.08
6	L	284	BPH	C4D-C3D-C2D	-4.76	100.94	107.08
6	L	284	BPH	O1D-CGD-CBD	-4.68	117.92	124.62
5	L	283	BCL	CMB-C2B-C1B	-4.48	120.95	128.36
5	M	310	BCL	CMB-C2B-C1B	-4.46	120.99	128.36
6	N	285	BPH	C4D-C3D-C2D	-4.43	101.37	107.08
7	N	286	U10	C7-C8-C9	-4.26	119.48	126.70
6	L	285	BPH	O1D-CGD-CBD	-4.15	118.67	124.62
5	M	309	BCL	CMB-C2B-C1B	-4.14	121.51	128.36
5	N	282	BCL	O1D-CGD-CBD	-4.11	118.73	124.62
5	M	310	BCL	O1D-CGD-CBD	-3.99	118.90	124.62
6	N	285	BPH	C7-C6-C5	-3.97	101.34	113.06
6	O	310	BPH	C4D-C3D-C2D	-3.88	102.07	107.08
5	L	282	BCL	CMB-C2B-C1B	-3.85	121.99	128.36
5	N	284	BCL	CMB-C2B-C1B	-3.56	122.48	128.36
7	N	286	U10	C36-C34-C33	-3.42	114.57	121.05
7	L	286	U10	C7-C8-C9	-3.36	121.00	126.70
6	N	285	BPH	OBD-CAD-C3D	-3.35	121.53	128.35
5	N	283	BCL	CMB-C2B-C1B	-3.31	122.89	128.36
5	N	283	BCL	O1D-CGD-CBD	-3.26	119.94	124.62
6	O	310	BPH	OBD-CAD-C3D	-3.22	121.78	128.35
5	N	284	BCL	OBD-CAD-C3D	-3.20	121.83	128.35
6	N	285	BPH	C1C-NC-C4C	-3.05	107.31	110.44
6	L	285	BPH	C6-C5-C3	-3.02	105.85	112.48
5	N	283	BCL	CBA-CAA-C2A	-3.00	105.26	113.73
5	L	282	BCL	CAC-C3C-C4C	-2.93	106.08	112.58
5	L	283	BCL	C6-C5-C3	-2.93	106.06	112.48
6	L	285	BPH	CAC-C3C-C2C	-2.92	106.79	114.13
5	N	284	BCL	CAA-C2A-C3A	-2.91	104.84	113.22
6	O	310	BPH	C1C-NC-C4C	-2.91	107.46	110.44
7	N	286	U10	C31-C32-C33	-2.90	104.08	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	282	BCL	CAC-C3C-C2C	-2.88	106.88	114.13
6	N	285	BPH	C17-C16-C15	-2.87	98.73	112.99
6	L	285	BPH	OBD-CAD-C3D	-2.85	122.55	128.35
6	L	284	BPH	OBD-CAD-C3D	-2.76	122.72	128.35
5	N	282	BCL	OBD-CAD-CBD	-2.72	121.83	125.94
5	M	310	BCL	CAC-C3C-C4C	-2.68	106.64	112.58
5	N	284	BCL	O1D-CGD-CBD	-2.63	120.85	124.62
5	N	282	BCL	CMB-C2B-C1B	-2.60	124.06	128.36
5	M	309	BCL	CAC-C3C-C4C	-2.57	106.88	112.58
5	L	283	BCL	OBD-CAD-C3D	-2.48	123.30	128.35
6	L	284	BPH	C4-C3-C2	-2.44	118.72	123.50
5	L	283	BCL	OBD-CAD-CBD	-2.37	122.36	125.94
6	L	285	BPH	CHC-C4B-NB	-2.33	120.47	124.91
5	O	309	BCL	O1D-CGD-CBD	-2.31	121.31	124.62
5	O	309	BCL	C4-C3-C2	-2.31	118.97	123.50
6	L	285	BPH	C4-C3-C2	-2.29	119.01	123.50
5	L	283	BCL	CAA-C2A-C3A	-2.25	106.76	113.22
7	O	311	U10	C37-C38-C39	-2.23	122.91	127.76
7	M	311	U10	C31-C32-C33	-2.23	105.86	111.69
5	O	309	BCL	OBD-CAD-C3D	-2.22	123.82	128.35
7	O	311	U10	C1-C6-C5	-2.20	117.61	120.12
5	N	283	BCL	OBD-CAD-C3D	-2.19	123.88	128.35
5	N	283	BCL	CAA-C2A-C3A	-2.19	106.92	113.22
5	N	283	BCL	C4-C3-C2	-2.17	119.24	123.50
7	L	286	U10	C11-C12-C13	-2.16	106.02	111.69
5	L	282	BCL	CAA-C2A-C3A	-2.15	107.03	113.22
5	M	309	BCL	OBD-CAD-C3D	-2.14	123.98	128.35
5	N	283	BCL	OBB-CAB-CBB	-2.13	115.03	120.13
5	M	310	BCL	OBD-CAD-C3D	-2.12	124.02	128.35
6	L	284	BPH	CAA-C2A-C3A	-2.11	107.15	113.22
7	L	286	U10	C50-C49-C48	-2.11	119.37	123.50
7	M	311	U10	C1M-C1-C6	-2.10	119.61	124.10
7	M	311	U10	C42-C43-C44	-2.10	123.20	127.76
5	L	282	BCL	CHA-C1A-NA	-2.10	120.90	126.06
5	N	284	BCL	CAC-C3C-C4C	-2.09	107.94	112.58
5	L	282	BCL	C7-C6-C5	-2.09	106.89	113.06
5	L	283	BCL	CMC-C2C-C3C	-2.08	105.13	114.35
6	L	284	BPH	CMA-C3A-C2A	-2.08	105.13	114.35
5	N	282	BCL	OBB-CAB-CBB	-2.06	115.19	120.13
5	O	309	BCL	CAC-C3C-C4C	-2.04	108.05	112.58
5	L	282	BCL	OBD-CAD-C3D	-2.02	124.22	128.35
5	L	283	BCL	CAC-C3C-C4C	-2.02	108.10	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	309	BCL	CMB-C2B-C1B	-2.01	125.04	128.36
7	M	311	U10	C50-C49-C48	-2.00	119.57	123.50
6	O	310	BPH	C14-C13-C12	2.00	118.77	111.08
6	L	284	BPH	C2A-C3A-C4A	2.00	105.68	101.10
5	N	283	BCL	C1D-CHD-C4C	2.02	129.15	126.07
5	M	309	BCL	CED-O2D-CGD	2.02	120.73	115.99
7	M	311	U10	C37-C36-C34	2.02	119.30	112.71
5	M	310	BCL	C2A-C1A-CHA	2.02	127.61	123.89
5	M	309	BCL	C4-C3-C5	2.04	118.52	115.41
5	N	284	BCL	CHD-C4C-NC	2.05	127.44	125.06
5	N	282	BCL	CMB-C2B-C3B	2.07	129.13	125.09
6	N	285	BPH	C16-C15-C13	2.08	122.39	115.49
7	M	311	U10	C40-C39-C41	2.08	118.59	115.41
6	L	285	BPH	C3A-C2A-C1A	2.09	104.49	101.84
7	O	311	U10	C3M-O3-C3	2.10	124.06	116.61
7	N	286	U10	C50-C49-C51	2.10	118.62	115.41
5	L	282	BCL	CBC-CAC-C3C	2.11	118.72	113.57
5	N	284	BCL	C4A-NA-C1A	2.12	109.10	106.36
5	N	283	BCL	C3A-C2A-C1A	2.12	105.10	101.50
6	L	285	BPH	C12-C11-C10	2.14	123.59	112.99
5	N	283	BCL	C2A-C1A-CHA	2.14	127.82	123.89
5	O	309	BCL	C4-C3-C5	2.18	118.74	115.41
6	O	310	BPH	CED-O2D-CGD	2.18	121.11	115.99
7	O	311	U10	C45-C44-C46	2.20	118.76	115.41
6	N	285	BPH	C11-C12-C13	2.20	122.78	115.49
5	M	309	BCL	CAA-CBA-CGA	2.20	119.77	113.32
6	L	285	BPH	C17-C16-C15	2.22	124.02	112.99
7	O	311	U10	C15-C14-C16	2.23	118.81	115.41
7	O	311	U10	C20-C19-C21	2.23	118.82	115.41
5	M	310	BCL	C4A-NA-C1A	2.24	109.26	106.36
6	L	285	BPH	CBA-CAA-C2A	2.25	120.07	113.73
6	N	285	BPH	CBA-CAA-C2A	2.25	120.07	113.73
7	L	286	U10	C56-C54-C55	2.27	120.21	114.64
7	O	311	U10	C50-C49-C51	2.29	118.91	115.41
5	N	284	BCL	C16-C17-C18	2.31	127.52	115.87
6	L	285	BPH	OBB-CAB-C3B	2.37	124.89	120.31
7	L	286	U10	C15-C14-C16	2.38	119.04	115.41
7	N	286	U10	C17-C16-C14	2.38	120.46	112.71
6	O	310	BPH	C11-C12-C13	2.41	123.49	115.49
5	O	309	BCL	CMB-C2B-C3B	2.43	129.84	125.09
7	M	311	U10	C4M-O4-C4	2.44	125.29	116.61
5	N	284	BCL	C4-C3-C5	2.47	119.19	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	284	BCL	CHB-C4A-NA	2.48	127.94	124.51
7	N	286	U10	C40-C39-C41	2.49	119.20	115.41
5	L	282	BCL	C4-C3-C5	2.52	119.25	115.41
5	L	282	BCL	CED-O2D-CGD	2.53	121.92	115.99
5	N	283	BCL	CBC-CAC-C3C	2.56	119.83	113.57
5	O	309	BCL	CED-O2D-CGD	2.57	122.01	115.99
5	M	309	BCL	O2A-CGA-CBA	2.58	119.75	111.90
5	N	283	BCL	O2A-CGA-CBA	2.59	119.80	111.90
7	M	311	U10	C35-C34-C36	2.61	119.40	115.41
5	M	310	BCL	CED-O2D-CGD	2.63	122.16	115.99
6	O	310	BPH	C11-C10-C8	2.63	124.22	115.49
5	N	282	BCL	CAA-CBA-CGA	2.64	121.05	113.32
5	N	282	BCL	O2A-CGA-CBA	2.76	120.32	111.90
7	L	286	U10	C45-C44-C46	2.88	119.81	115.41
7	O	311	U10	C35-C34-C36	2.89	119.82	115.41
7	L	286	U10	C40-C39-C41	2.90	119.84	115.41
5	L	283	BCL	O2D-CGD-CBD	2.93	115.31	111.30
5	L	283	BCL	C4-C3-C5	2.93	119.88	115.41
7	M	311	U10	C50-C49-C51	2.95	119.91	115.41
5	L	282	BCL	C3D-CAD-CBD	2.95	111.77	107.60
5	N	283	BCL	CMB-C2B-C3B	2.99	130.94	125.09
7	M	311	U10	C10-C9-C11	3.07	120.09	115.41
6	L	285	BPH	CED-O2D-CGD	3.12	123.30	115.99
7	L	286	U10	C20-C19-C21	3.12	120.18	115.41
6	O	310	BPH	C4-C3-C5	3.17	120.24	115.41
7	O	311	U10	C40-C39-C41	3.17	120.25	115.41
5	M	310	BCL	C3D-CAD-CBD	3.22	112.15	107.60
5	L	283	BCL	CAA-CBA-CGA	3.32	123.03	113.32
5	L	282	BCL	CMB-C2B-C3B	3.33	131.59	125.09
5	N	284	BCL	C3D-CAD-CBD	3.33	112.31	107.60
5	N	284	BCL	CMB-C2B-C3B	3.35	131.63	125.09
5	N	284	BCL	CED-O2D-CGD	3.35	123.84	115.99
5	N	282	BCL	C3D-CAD-CBD	3.39	112.39	107.60
7	N	286	U10	C8-C7-C6	3.41	121.89	111.64
7	M	311	U10	C30-C29-C31	3.42	120.62	115.41
5	M	309	BCL	CBA-CAA-C2A	3.42	123.38	113.73
5	N	284	BCL	CAA-CBA-CGA	3.43	123.37	113.32
5	M	309	BCL	C11-C12-C13	3.44	126.90	115.49
7	L	286	U10	C50-C49-C51	3.45	120.68	115.41
6	N	285	BPH	C4-C3-C5	3.49	120.74	115.41
6	O	310	BPH	C3D-CAD-CBD	3.55	112.61	107.60
6	L	285	BPH	C4-C3-C5	3.57	120.86	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	309	BCL	C3D-CAD-CBD	3.59	112.67	107.60
5	O	309	BCL	C3D-CAD-CBD	3.64	112.75	107.60
6	N	285	BPH	C3D-CAD-CBD	3.67	112.79	107.60
5	M	309	BCL	CMB-C2B-C3B	3.68	132.29	125.09
5	N	283	BCL	C4-C3-C5	3.73	121.10	115.41
5	N	283	BCL	C3D-CAD-CBD	3.80	112.96	107.60
5	N	283	BCL	O2D-CGD-CBD	3.82	116.54	111.30
6	L	284	BPH	C4-C3-C5	4.06	121.61	115.41
5	M	310	BCL	CMB-C2B-C3B	4.09	133.09	125.09
6	O	310	BPH	C3C-C4C-NC	4.17	112.11	107.93
6	L	284	BPH	C3D-CAD-CBD	4.17	113.49	107.60
5	L	283	BCL	CMB-C2B-C3B	4.22	133.34	125.09
6	L	285	BPH	C3C-C4C-NC	4.32	112.26	107.93
6	L	285	BPH	O2D-CGD-CBD	4.68	117.72	111.30
6	L	285	BPH	C3D-CAD-CBD	4.72	114.26	107.60
5	L	283	BCL	C3D-CAD-CBD	4.75	114.31	107.60
7	N	286	U10	C7-C6-C5	4.78	124.18	118.56
6	L	284	BPH	C3C-C4C-NC	4.84	112.78	107.93
5	M	310	BCL	O2D-CGD-CBD	4.85	117.95	111.30
5	O	309	BCL	O2D-CGD-CBD	4.94	118.08	111.30
5	N	282	BCL	O2D-CGD-CBD	5.26	118.52	111.30
7	N	286	U10	C35-C34-C36	5.37	123.61	115.41
5	M	309	BCL	O2D-CGD-CBD	5.51	118.86	111.30
6	L	284	BPH	O2D-CGD-CBD	5.65	119.04	111.30
6	N	285	BPH	C3C-C4C-NC	5.78	113.72	107.93
5	N	282	BCL	CBA-CAA-C2A	5.97	130.57	113.73
6	O	310	BPH	O2D-CGD-CBD	7.39	121.44	111.30
6	N	285	BPH	O2D-CGD-CBD	7.58	121.70	111.30

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	O	310	BPH	C13
6	L	284	BPH	C8
6	L	284	BPH	C13
6	N	285	BPH	C8
5	O	309	BCL	C8
6	L	285	BPH	C8
5	M	310	BCL	C8
5	M	310	BCL	C13
5	N	282	BCL	C8
5	N	282	BCL	C13

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Mol	Chain	Res	Type	Atom
5	M	309	BCL	C8
5	M	309	BCL	C13

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	282	BCL	8	0
5	L	283	BCL	6	0
6	L	284	BPH	2	0
6	L	285	BPH	9	0
7	L	286	U10	4	0
5	M	309	BCL	7	0
5	M	310	BCL	5	0
7	M	311	U10	1	0
5	N	282	BCL	7	0
5	N	283	BCL	6	0
5	N	284	BCL	7	0
6	N	285	BPH	7	0
7	N	286	U10	6	0
5	O	309	BCL	9	0
6	O	310	BPH	3	0
7	O	311	U10	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.